

10521972.trn

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Welcome to STN International! Enter x:x

LOGINID : SSSPTA1626GMS

PASSWORD :

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * * * * Welcome to STN International * * * * * * * * * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 JAN 08 CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 3 JAN 16 CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 4 JAN 16 IPC version 2007.01 thesaurus available on STN
NEWS 5 JAN 16 WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 6 JAN 22 CA/CAplus updated with revised CAS roles
NEWS 7 JAN 22 CA/CAplus enhanced with patent applications from India
NEWS 8 JAN 29 PHAR reloaded with new search and display fields
NEWS 9 JAN 29 CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 10 FEB 15 PATDPASPC enhanced with Drug Approval numbers
NEWS 11 FEB 15 RUSSIAPAT enhanced with pre-1994 records
NEWS 12 FEB 23 KOREAPAT enhanced with IPC 8 features and functionality
NEWS 13 FEB 26 MEDLINE reloaded with enhancements
NEWS 14 FEB 26 EMBASE enhanced with Clinical Trial Number field
NEWS 15 FEB 26 TOXCENTER enhanced with reloaded MEDLINE
NEWS 16 FEB 26 IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 17 FEB 26 CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases.
NEWS 18 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 19 MAR 16 CASREACT coverage extended
NEWS 20 MAR 20 MARPAT now updated daily
NEWS 21 MAR 22 LWPI reloaded
NEWS 22 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 23 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 24 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 25 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 26 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 27 APR 30 INPADOC replaced by INPADOCDB on STN
NEWS 28 MAY 01 New CAS web site launched
NEWS 29 MAY 08 CA/CAplus Indian patent publication number format defined

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 13:08:04 ON 10 MAY 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT F

Do you want t

Choice (Y/n) :

Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE
ENTRY | TOTAL
SESSION |
|----------------------|---------------------|------------------|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 13:08:18 ON 10 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by ICS Chem3D Pro.

STRUCTURE FILE UPDATES: 9 MAY 2007 HIGHEST RN 934521-72-9
DICTIONARY FILE UPDATES: 9 MAY 2007 HIGHEST RN 934521-72-9

NW GAS Information Use Policies - section HELP WISCONSIN'S SMALL BUSINESSES

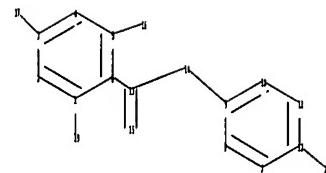
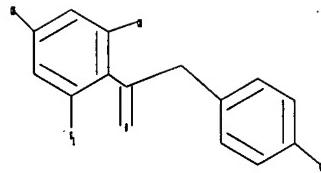
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2021

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY refer to:

<http://www.cas.org/support/stndgen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10521972.str



```

chain nodes :
13 14 15 16 17 19 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
1-19 3-17 5-16 6-13 9-14 12-21 13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
1-19 3-17 5-16 12-21 13-15
exact bonds :
6-13 9-14 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1 : 7 :

```

G1:H,OH

G2:OH,MeO,EtO,n-PrO,n-BuO

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS
21:CLASS

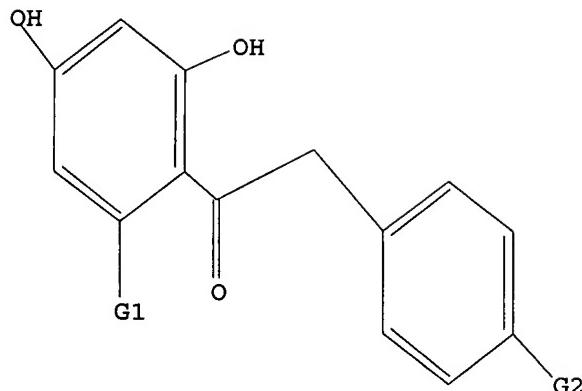
```

L1 STRUCTURE UPLOADED

```

=> d 11
L1 HAS NO ANSWERS
L1 STR

```



G1 H, OH

G2 OH, MeO, EtO, n-PrO, n-BuO

Structure attributes must be viewed using STN Express query preparation.

```
=> s 11
SAMPLE SEARCH INITIATED 13:08:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 114 TO ITERATE

100.0% PROCESSED      114 ITERATIONS           11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:    1640 TO     2920
PROJECTED ANSWERS:        22 TO      418

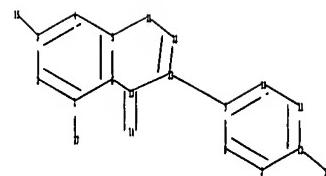
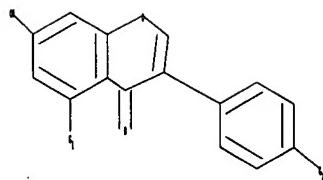
L2      11 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 13:08:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2486 TO ITERATE

100.0% PROCESSED      2486 ITERATIONS           195 ANSWERS
SEARCH TIME: 00.00.01

L3      195 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10521972a.str
```



chain nodes :

14 15 17 19

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 21 22 23

chain bonds :

1-17 3-15 9-23 12-19 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-21 6-13 7-8 7-12 8-9 9-10 10-11 11-12 13-23
21-22 22-23

exact/norm bonds :

1-17 3-15 12-19 13-14

exact bonds :

5-21 6-13 9-23 13-23 21-22 22-23

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

G1:H,OH

G2:OH,MeO,EtO,n-PrO,n-BuO

Match level :

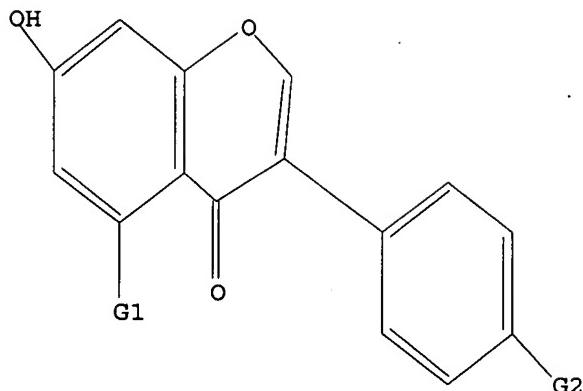
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 17:CLASS 19:CLASS 21:CLASS
22:Atom 23:Atom

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR



G1 H, OH

G2 OH, MeO, EtO, n-PrO, n-BuO

Structure attributes must be viewed using STN Express query preparation.

```
=> s 14
SAMPLE SEARCH INITIATED 13:11:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 793 TO ITERATE

100.0% PROCESSED      793 ITERATIONS          40 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:    14171 TO    17549
PROJECTED ANSWERS:       421 TO     1179

L5      40 SEA SSS SAM L4

=> s 14 sss full
FULL SEARCH INITIATED 13:11:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 15967 TO ITERATE

100.0% PROCESSED      15967 ITERATIONS          897 ANSWERS
SEARCH TIME: 00.00.01
```

L6 897 SEA SSS FUL L4

```
=>
Uploading C:\Program Files\Stnexp\Queries\10521972b.str
```



chain nodes :

3 4 5 6 7 8 9

chain bonds :

3-4 4-5 4-8 5-6 6-7 6-9

10521972.trn

exact/norm bonds :
4-5 4-8 5-6 6-7 6-9
exact bonds :
3-4

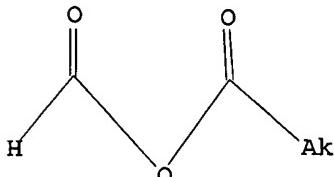
G1:H,OH

G2:OH,MeO,EtO,n-PrO,n-BuO

Match level :
3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L7 STRUCTURE UPLOADED

=> d 17
L7 HAS NO ANSWERS
L7 STR



G1 H,OH

G2 OH,MeO,EtO,n-PrO,n-BuO

Structure attributes must be viewed using STN Express query preparation.

=> s 17
SAMPLE SEARCH INITIATED 13:16:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 7792 TO ITERATE

25.7% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 150549 TO 161131
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s 17 sss full
FULL SEARCH INITIATED 13:17:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 154780 TO ITERATE

100.0% PROCESSED 154780 ITERATIONS 40 ANSWERS
SEARCH TIME: 00.00.02

L9 40 SEA SSS FUL L7

10521972.trn

=> FIL HCAPLUS
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 521.70 | 521.91 |

FILE 'HCAPLUS' ENTERED AT 13:17:09 ON 10 MAY 2007
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FILE COVERS 1907 - 10 May 2007 VOL ISS ISS
FILE LAST UPDATED: 9 May 2007 (20070509/ED)
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FILE COVERS 1907 - 10 May 2007 VOL 146 ISS 20
FILE LAST UPDATED: 1 May 2007 (20070501/ED)

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This file contains CAS Registry Numbers for easy and accurate

=> d his

(FILE 'HOME' ENTERED AT 13:08:04 ON 10 MAY 2007)

FILE 'REGISTRY' ENTERED AT 13:08:18 ON 10 MAY 2007
L1 STRUCTURE UPLOADED
L2 11 S L1
L3 195 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 40 S L4
L6 897 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 0 S L7
L9 40 S L7 SSS FULL

FILE 'HCAPLUS' ENTERED AT 13:17:09 ON 10 MAY 2007

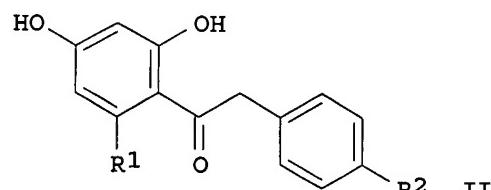
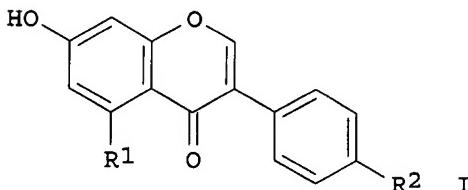
=> s l3
L10 557 L3
=> s 16
L11 8900 L6
=> s 19
L12 405 L9
=> s 110 and 112
L13 8 L10 AND L12
=> s 110 and 111
L14 380 L10 AND L11

```
=> s l11 and l12  
L15          8 L11 AND L12  
  
=> d l13 ibib abs hitstr tot
```

L13 ANSWER 1 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|---|----------|-----------------|------------|
| WO 2004009576 | A2 | 20040129 | WO 2003-EP7575 | 20030714 |
| WO 2004009576 | A3 | 20040513 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ,
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| CA 2492201 | A1 | 20040129 | CA 2003-2492201 | 20030714 |
| AU 2003254341 | A1 | 20040209 | AU 2003-254341 | 20030714 |
| EP 1523478 | A2 | 20050420 | EP 2003-764976 | 20030714 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | |
| BR 2003012840 | A | 20050426 | BR 2003-12840 | 20030714 |
| CN 1684950 | A | 20051019 | CN 2003-817676 | 20030714 |
| JP 2005534682 | T | 20051117 | JP 2004-522445 | 20030714 |
| US 2005256321 | A1 | 20051117 | US 2005-521972 | 20050121 |
| PRIORITY APPLN. INFO.: | | | EP 2002-16494 | A 20020723 |
| | | | WO 2003-EP7575 | W 20030714 |
| OTHER SOURCE(S) | | | | |

OTHER SOURCE(S) : CASREACT 140:128190; MARPAT 140:128190
GI



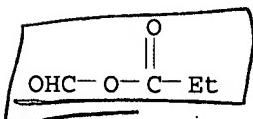
AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR3 [R3 = alkyl, haloalkyl, alkoxyethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.

IT 10500-31-9P, Propionyl formic anhydride

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)

RN 10500-31-9 HCAPLUS

CN Propanoic acid, anhydride with formic acid (9CI) (CA INDEX NAME)

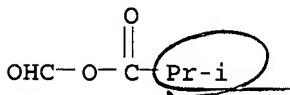


IT 10500-33-1, Isobutyric formic anhydride 15485-65-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)

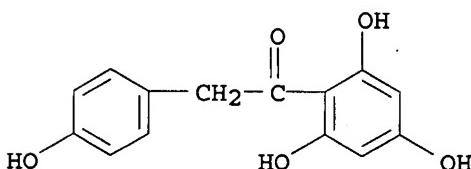
RN 10500-33-1 HCAPLUS

CN Propanoic acid, 2-methyl-, anhydride with formic acid (9CI) (CA INDEX NAME)



RN 15485-65-1 HCAPLUS

CN Ethanone, 2-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME)



L13 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:832777 HCAPLUS

DOCUMENT NUMBER: 137:337726

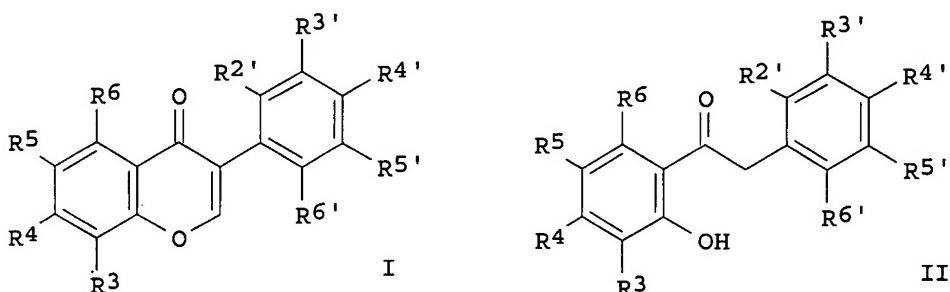
TITLE: Process for preparing isoflavone derivatives from 2-hydroxyaryl alkyl ketones in the presence of formic-sulfuric anhydride salt

INVENTOR(S) : Burdick, David Carl
 PATENT ASSIGNEE(S) : Roche Vitamins A.-G., Switz.
 SOURCE: PCT Int. Appl., 15 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2002085881 | A1 | 20021031 | WO 2002-EP4319 | 20020419 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2443431 | A1 | 20021031 | CA 2002-2443431 | 20020419 |
| AU 2002338399 | A1 | 20021105 | AU 2002-338399 | 20020419 |
| EP 1392671 | A1 | 20040303 | EP 2002-742905 | 20020419 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2002009157 | A | 20040608 | BR 2002-9157 | 20020419 |
| CN 1505621 | A | 20040616 | CN 2002-808879 | 20020419 |
| JP 2004526784 | T | 20040902 | JP 2002-583408 | 20020419 |
| US 2004158082 | A1 | 20040812 | US 2004-474418 | 20040311 |
| US 7109358 | B2 | 20060919 | | |

PRIORITY APPLN. INFO.:

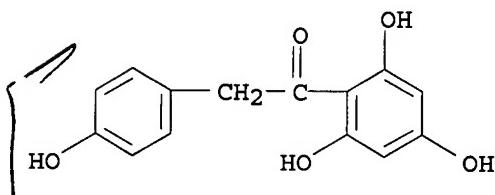
OTHER SOURCE(S) : CASREACT 137:337726; MARPAT 137:337726
 GI



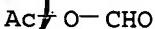
AB The invention relates to a process for preparing isoflavone derivs., such as I [R₃ = H, OH, alkyl; R₄ = H, OH, alkoxy; R₅, R₆, R_{2'}, R_{3'}, R_{5'}, R_{6'} = H, OH, alkoxy, alkyl; R_{4'} = H, OH, alkoxy], from 2-hydroxyaryl alkyl ketone (II) in the presence of a base with formic-sulfuric anhydride salt, such as (HCOOSO₃)_nX_n [X = metallic cation, ammonium, amine salt, heterocyclic base, quaternary ammonium, phosphonium salt including polymeric or polymer bound forms thereof; n = 1-4]. Thus, reaction between sodium formylsulfate (prepared in situ by the reaction of sodium formate and sulfur

trioxide-dimethylformamide complex) and 2,4,6-trihydroxyphenyl-4'-hydroxybenzyl ketone afforded genistein (5,7,4'-trihydroxyisoflavone) in 95% yield.

- IT 15485-65-1, 2,4,6-Trihydroxyphenyl-4'-hydroxybenzyl ketone
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of isoflavones from (2-hydroxyaryl) alkyl ketones in the presence of formic-sulfuric anhydride salt)
- RN 15485-65-1 HCPLUS
- CN Ethanone, 2-(4-hydroxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME)

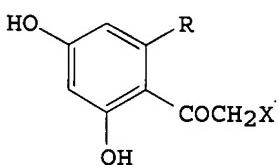


- IT 2258-42-6P, Formic acetic anhydride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of isoflavones from (2-hydroxyaryl) alkyl ketones in the presence of formic-sulfuric anhydride salt)
- RN 2258-42-6 HCPLUS
- CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

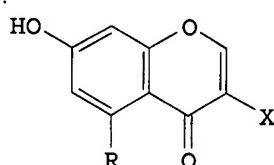


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:212822 HCPLUS
 DOCUMENT NUMBER: 118:212822
 TITLE: Formic acetic anhydride in the synthesis of chromones.
 2. Synthesis of 3-arylchromones
 AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.
 CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, Ukraine
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (5), 595-600
 CODEN: KGSSAQ; ISSN: 0132-6244
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 118:212822
 GI



I



II

AB Dihydroxyphenylacetophenone I (R = H, X = Ph) underwent cyclization to

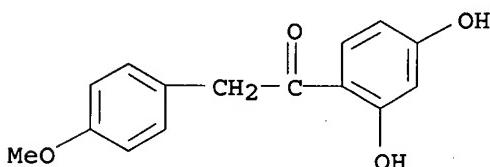
arylchromone II (near quant. yield) in reaction with HCO₂Ac via initial formylation of I under mild conditions, followed by base-catalyzed cyclization. Trialkylamines were the most effective cyclization catalysts. Et₃N catalyzed the cyclization of other I derivs. (R = H, OH; X = e.g., substituted Ph or furyl) to II. The cyclization is most effectively applied to preparation of II containing electron-withdrawing X groups.

IT 487-49-0 15485-66-2 17720-60-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(heterocyclization of, with formic acetic anhydride,
trialkylamine-catalyzed)

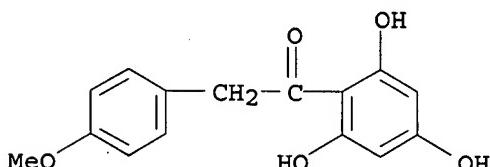
RN 487-49-0 HCPLUS

CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



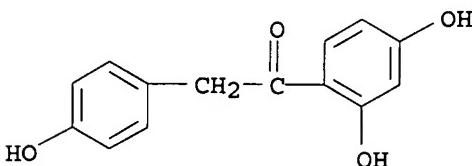
RN 15485-66-2 HCPLUS

CN Ethanone, 2-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME).



RN 17720-60-4 HCPLUS

CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



IT 2258-42-6, Formic acetic anhydride

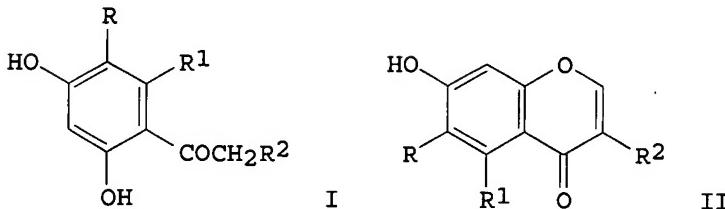
RL: RCT (Reactant); RACT (Reactant or reagent)
(heterocyclization reaction of, with hydroxyacetophenones,
trialkylamine-catalyzed)

RN 2258-42-6 HCPLUS

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

L13 ANSWER 4 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1992:20893 HCPLUS
 DOCUMENT NUMBER: 116:20893
 TITLE: Formic acetic anhydride in the synthesis of chromones.
 AUTHOR(S): 1. Synthesis of 3-heteroarylchromones
 Pivovarenko, V. G.; Khilya, V. P.
 CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, USSR
 SOURCE: Khimiya Geterotsiklichesikh Soedinenii (1991), (5),
 625-31
 DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0453-8234
 Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 116:20893
 GI



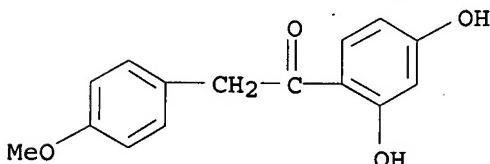
AB The reaction of hetarylacetophenones I ($R = H, Me, Pr, 1\text{-hexyl}$; $R1 = H, OH, CO_2H$; $R2 = \text{azolyl, substituted Ph}$) with HCO_2COMe gives, under HCO_2Na catalysis, chromones II. The yield of II and the reaction rate increase with increasing π -deficiency of the hetaryl substituent or with the presence of an OH group in the C6 position of the starting acetophenone. II ($R2 = \text{azolyl}$) are formed even in the absence of catalyst.

IT 487-49-0 15485-66-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with formic acetic anhydride)

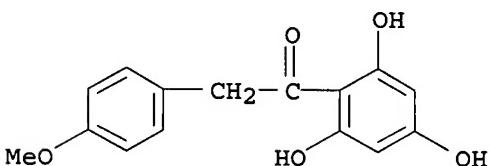
RN 487-49-0 HCPLUS

CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 15485-66-2 HCPLUS

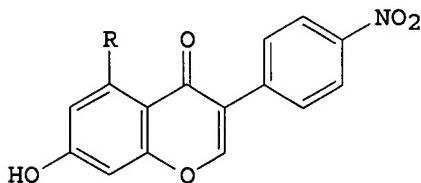
CN Ethanone, 2-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME)



IT 2258-42-6P, Formic acetic anhydride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and cyclocondensation of, with hetarylacetophenones)
 RN 2258-42-6 HCPLUS
 CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

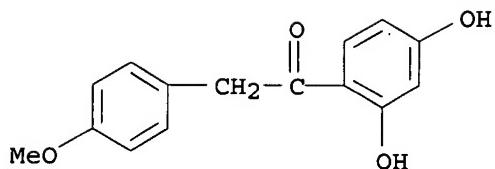
L13 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1992:6375 HCPLUS
 DOCUMENT NUMBER: 116:6375
 TITLE: A facile and practical preparation of
 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one
 AUTHOR(S): Liu, D. F.; Cheng, C. C.
 CORPORATE SOURCE: Cancer Cent., Univ. Kansas, Kansas City, KS, 66103,
 USA
 SOURCE: Journal of Heterocyclic Chemistry (1991), 28(6),
 1641-2
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 116:6375
 GI



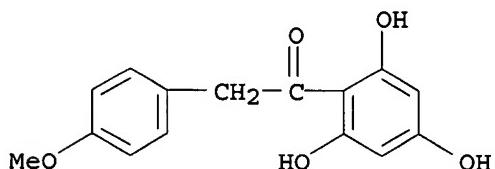
AB In spite of the fact that several preparative methods for the synthesis of hydroxylated isoflavones were reported during the past fifty years, none is suitable for the preparation of isoflavones containing 5,7-dihydroxy functions.

This paper reports a simple, large scale preparation of 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one (I, R = OH) by the condensation of the readily available 2,4,6-(HO)3C6H2COCH2C6H4NO2-4 and acetic formic anhydride in high yields. Similar isoflavones, such as I (R = H), can also be obtained in good yields in an analogous manner.

IT 487-49-0 15485-66-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with acetic formic anhydride)
 RN 487-49-0 HCPLUS
 CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



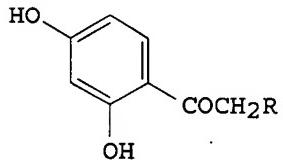
RN 15485-66-2 HCPLUS
 CN Ethanone, 2-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME)



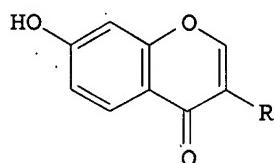
IT 2258-42-6P, Acetic formic anhydride
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (formation and cyclocondensation of, with phenyl(hydroxyphenyl)ethanone
 s)
 RN 2258-42-6 HCPLUS
 CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

L13 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:405988 HCPLUS
 DOCUMENT NUMBER: 113:5988
 TITLE: Simple and effective synthesis of isoflavones and
 3-arylhydroxychromones
 AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Vasil'ev, S. A.
 CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, USSR
 SOURCE: Khimiya Prirodnnykh Soedinenii (1989), (5), 639-43
 CODEN: KPSUAR; ISSN: 0023-1150
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 113:5988
 GI



I



II

AB Cyclocondensation of acetophenones I (R = substituted Ph, PhO, p-FC₆H₄O) with MeCO₂CHO, prepared from HCO₂H and CH₂:C:O, gave 15-99% isoflavones II. Similarly, I react with the Vilsmeier reagent to give 95.7-98.5% II.

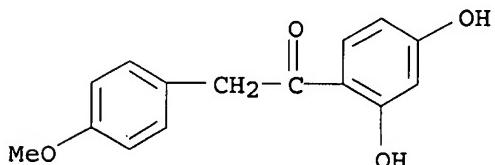
10521972.trn

IT 487-49-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with formicacetic anhydride or Vilsmeier
reagent, isoflavone from)

RN 487-49-0 HCPLUS

CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX
NAME)



IT 2258-42-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclocondensation with hydroxyacetophenones, isoflavones
from)

RN 2258-42-6 HCPLUS

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

L13 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:129748 HCPLUS

DOCUMENT NUMBER: 104:129748

TITLE: Synthesis of 5,7-dihydroxyisoflavones and their
heterocyclic analogs using acetoformic anhydride

AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.

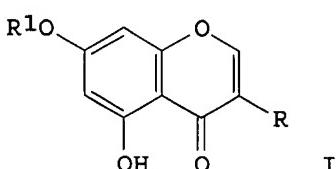
CORPORATE SOURCE: Kiiv. Derzh. Univ., Kiev, USSR

SOURCE: Dopovid Akademii Nauk Ukrains'koi RSR, Seriya B:
Geologichni, Khimichni ta Biologichni Nauki (1985),
(7), 44-7

DOCUMENT TYPE: CODEN: DANND6; ISSN: 0377-9785

LANGUAGE: Journal

GI Ukrainian



AB 2,4,6-(HO)3C6H2COCH2R [R = 2-pyridyl, 2-quinolyl, 2-methyl-4-thiazolyl,
5-(ethoxycarbonyl)-2-furyl, p-ClC6H4, o- and p-FC6H4, p-MeOC6H4,
dihydro-6-benzodioxinyl] cyclized in the presence of HCO2Ac and either
HCO2Na or Et3N to give the corresponding chromones I (R1 = H) in
≤100% yield. The intermediate I (R = heterocyclyl, R1 = HCO) were
also isolated.

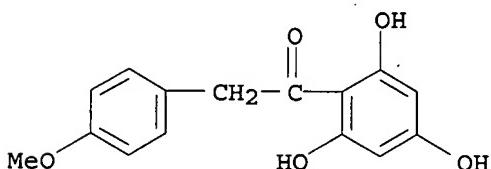
10521972.trn

IT 15485-66-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with acetoformic anhydride)

RN 15485-66-2 HCPLUS

CN Ethanone, 2-(4-methoxyphenyl)-1-(2,4,6-trihydroxyphenyl)- (CA INDEX NAME)



IT 2258-42-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization with, of aryltrihydroxyacetophenones)

RN 2258-42-6 HCPLUS

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

L13 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:541792 HCPLUS

DOCUMENT NUMBER: 103:141792

TITLE: Acetic formic anhydride as a cyclizing reagent in the synthesis of isoflavones and 3-hetarylchromones

AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Babichev, F. S.

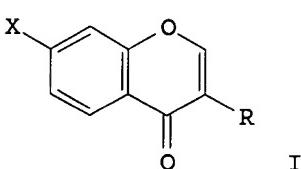
CORPORATE SOURCE: Kiv. Derzh. Univ., Kiev, USSR

SOURCE: Dopovid Akademii Nauk Ukrains'koi RSR, Seriya B: Geologichni, Khimichni ta Biologichni Nauki (1985), (4), 56-9

DOCUMENT TYPE: CODEN: DANND6; ISSN: 0377-9785

LANGUAGE: Journal

GI Ukrainian



AB HCO₂Ac catalyzed the cyclization of 2,4-(HO)C₈H₄COCH₂R [R = 2-pyridyl, 2- and 7-quinolyl, 2-methyl-4-thiazolyl, 5-(ethoxycarbonyl)-2-furyl, C₆H₄NO₂-4, Ph, C₆H₄OMe-4, Me] in the presence of NaO₂CH or Et₃N to give ≤99% chromones I (X = HO, same R). The intermediate I (X = HCO₂; R = 2-pyridyl, 2-quinolyl, 2-methyl-4-thiazolyl) were also isolated.

IT 2258-42-6

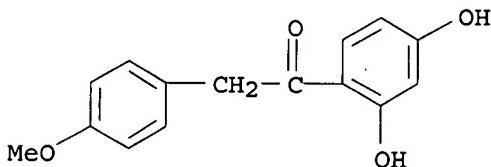
RL: CAT (Catalyst use); USES (Uses)
(catalysts, with base, for cyclization of dihydroxyacetophenones to chromones)

10521972.trn

RN 2258-42-6 HCAPLUS
CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

IT 487-49-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, chromone by, catalysts for)
RN 487-49-0 HCAPLUS
CN Ethanone, 1-(2,4-dihydroxyphenyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

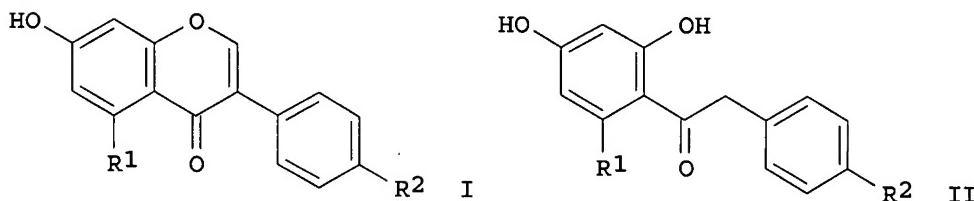


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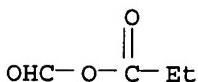
L15 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80674 HCAPLUS
DOCUMENT NUMBER: 140:128190
TITLE: Process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivatives
INVENTOR(S): Burdet, Bruno; Ruettimann, August
PATENT ASSIGNEE(S): Roche Vitamins Ag, Switz.; DSM IP Assets B.V.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------|
| WO 2004009576 | A2 | 20040129 | WO 2003-EP7575 | 20030714 |
| WO 2004009576 | A3 | 20040513 | | |
| W: | AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW | | | |
| RW: | GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | |
| CA 2492201 | A1 | 20040129 | CA 2003-2492201 | 20030714 |
| AU 2003254341 | A1 | 20040209 | AU 2003-254341 | 20030714 |
| EP 1523478 | A2 | 20050420 | EP 2003-764976 | 20030714 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | |

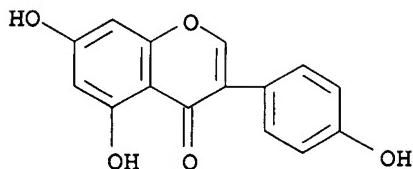
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
 BR 2003012840 A 20050426 BR 2003-12840 20030714
 CN 1684950 A 20051019 CN 2003-817676 20030714
 JP 2005534682 T 20051117 JP 2004-522445 20030714
 US 2005256321 A1 20051117 US 2005-521972 20050121
 PRIORITY APPLN. INFO.: EP 2002-16494 A 20020723
 OTHER SOURCE(S): WO 2003-EP7575 W 20030714
 GI CASREACT 140:128190; MARPAT 140:128190



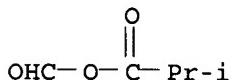
- AB The present invention discloses a process for manufacturing hydroxylated isoflavone derivs., such as I [R1 = H, OH; R2 = OH, alkoxy] by reacting an appropriately substituted 2-hydroxydeoxybenzoin derivs. II with formic acid anhydride, HCOOCOR₃ [R₃ = alkyl, haloalkyl, alkoxymethyl, carboxyalkyl, arylalkyl, cycloalkyl, aryl, heteroaryl, aminoalkyl, alkoxy, aryloxy], in the presence of a base or in a solvent which acts as a base, and if necessary promoting the ensuing hydrolysis of the so-produced acylated form of I by acidification. Of particular interest as products of this process are the 5,7-dihydroxyisoflavones, e.g. genistein I [R1, R2 = OH (III)]. Thus, propionyl formic anhydride, formed by the reaction of sodium formate and propionyl chloride, was reacted with II [R1, R2 = OH], and the product was hydrolyzed to afford III of 98.9% purity. Isoflavones display many useful biochem. effects.
- IT 10500-31-9P, Propionyl formic anhydride
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)
- RN 10500-31-9 HCPLUS
- CN Propanoic acid, anhydride with formic acid (9CI) (CA INDEX NAME)



- IT 446-72-0P, Genistein
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (process for manufacturing hydroxylated isoflavones by reacting 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)
- RN 446-72-0 HCPLUS
- CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (CA INDEX NAME)



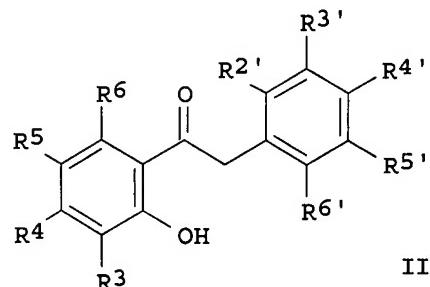
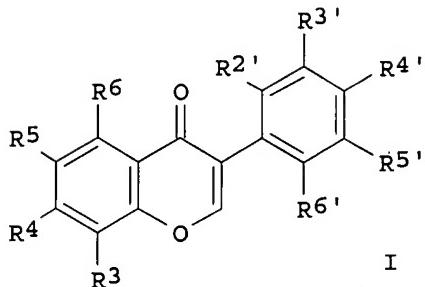
IT 10500-33-1, Isobutyric formic anhydride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process for manufacturing hydroxylated isoflavones by reacting
 2-hydroxydeoxybenzoins with formic acid anhydride derivs.)
 RN 10500-33-1 HCAPLUS
 CN Propanoic acid, 2-methyl-, anhydride with formic acid (9CI) (CA INDEX
 NAME)



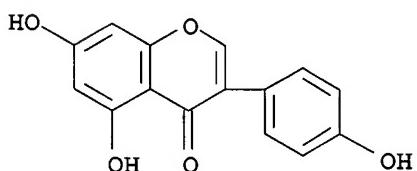
L15 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:832777 HCAPLUS
 DOCUMENT NUMBER: 137:337726
 TITLE: Process for preparing isoflavone derivatives from
 2-hydroxyaryl alkyl ketones in the presence of
 formic-sulfuric anhydride salt
 INVENTOR(S): Burdick, David Carl
 PATENT ASSIGNEE(S): Roche Vitamins A.-G., Switz.
 SOURCE: PCT Int. Appl., 15 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|----------|
| WO 2002085881 | A1 | 20021031 | WO 2002-EP4319 | 20020419 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2443431 | A1 | 20021031 | CA 2002-2443431 | 20020419 |
| AU 2002338399 | A1 | 20021105 | AU 2002-338399 | 20020419 |
| EP 1392671 | A1 | 20040303 | EP 2002-742905 | 20020419 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2002009157 | A | 20040608 | BR 2002-9157 | 20020419 |
| CN 1505621 | A | 20040616 | CN 2002-808879 | 20020419 |
| JP 2004526784 | T | 20040902 | JP 2002-583408 | 20020419 |
| US 2004158082 | A1 | 20040812 | US 2004-474418 | 20040311 |

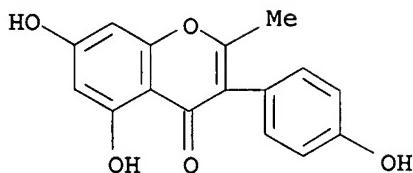
US 7109358 B2 20060919 EP 2001-110212 A 20010425
 PRIORITY APPLN. INFO.: WO 2002-EP4319 W 20020419
 OTHER SOURCE(S): CASREACT 137:337726; MARPAT 137:337726
 GI



- AB The invention relates to a process for preparing isoflavone derivs., such as I [R3 = H, OH, alkyl; R4 = H, OH, alkoxy; R5, R6, R2', R3', R5', R6' = H, OH, alkoxy, alkyl; R4' = H, OH, alkoxy], from 2-hydroxyaryl alkyl ketone (II) in the presence of a base with formic-sulfuric anhydride salt, such as (HCOOSO₃)_nX_n [X = metallic cation, ammonium, amine salt, heterocyclic base, quaternary ammonium, phosphonium salt including polymeric or polymer bound forms thereof; n = 1-4]. Thus, reaction between sodium formylsulfate (prepared in situ by the reaction of sodium formate and sulfur trioxide-dimethylformamide complex) and 2,4,6-trihydroxyphenyl-4'-hydroxybenzyl ketone afforded genistein (5,7,4'-trihydroxyisoflavone) in 95% yield.
- IT 446-72-0P, Genistein 121324-24-1P, 2-Methylgenistein
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
 (preparation of isoflavones from (2-hydroxyaryl) alkyl ketones in the presence of formic-sulfuric anhydride salt)
- RN 446-72-0 HCPLUS
- CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (CA INDEX NAME)



- RN 121324-24-1 HCPLUS
- CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)-2-methyl- (9CI)
 (CA INDEX NAME)

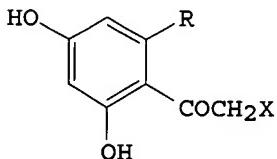


IT 2258-42-6P, Formic acetic anhydride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of isoflavones from (2-hydroxyaryl) alkyl ketones in the presence of formic-sulfuric anhydride salt)
 RN 2258-42-6 HCAPLUS
 CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

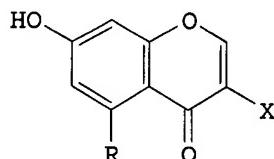
Ac—O—CHO

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1993:212822 HCAPLUS
 DOCUMENT NUMBER: 118:212822
 TITLE: Formic acetic anhydride in the synthesis of chromones.
 2. Synthesis of 3-arylchromones
 AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.
 CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, Ukraine
 SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1992), (5), 595-600
 DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0132-6244
 LANGUAGE: Journal
 Russian
 OTHER SOURCE(S): CASREACT 118:212822
 GI



I



II

AB Dihydroxyphenylacetophenone I ($R = H, X = Ph$) underwent cyclization to arylchromone II (near quant. yield) in reaction with HCO_2Ac via initial formylation of I under mild conditions, followed by base-catalyzed cyclization. Trialkylamines were the most effective cyclization catalysts. Et_3N catalyzed the cyclization of other I derivs. ($R = H, OH; X = e.g.,$ substituted Ph or furyl) to II. The cyclization is most effectively applied to preparation of II containing electron-withdrawing X groups.

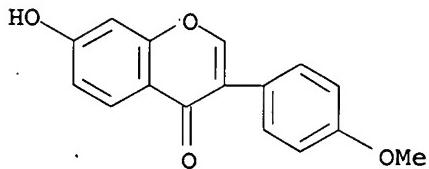
IT 2258-42-6, Formic acetic anhydride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (heterocyclization reaction of, with hydroxyacetophenones,

10521972.trn

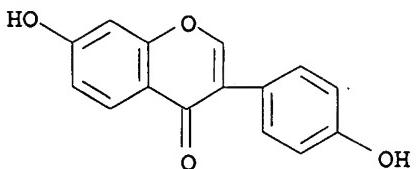
trialkylamine-catalyzed)
RN 2258-42-6 HCPLUS
CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

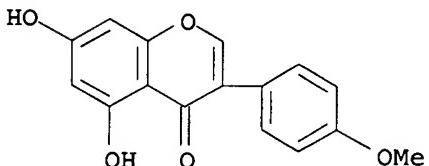
IT 485-72-3P 486-66-8P 491-80-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 485-72-3 HCPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



RN 486-66-8 HCPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (CA INDEX NAME)



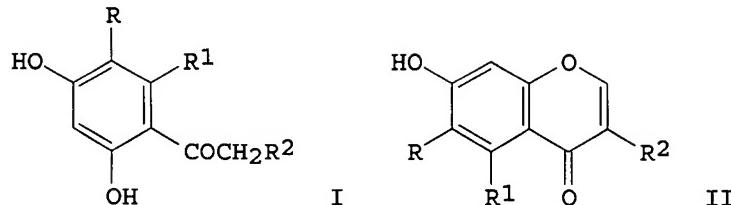
RN 491-80-5 HCPLUS
CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



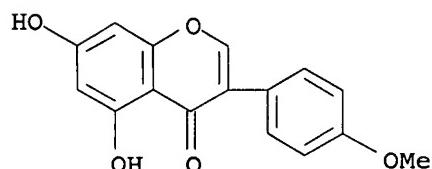
L15 ANSWER 4 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:20893 HCPLUS
DOCUMENT NUMBER: 116:20893
TITLE: Formic acetic anhydride in the synthesis of chromones.
1. Synthesis of 3-heteroarylchromones
AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.
CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, 252017, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1991), (5),
625-31
DOCUMENT TYPE: CODEN: KGSSAQ; ISSN: 0453-8234
LANGUAGE: Journal
Russian

OTHER SOURCE(S) :
GI

CASREACT 116:20893



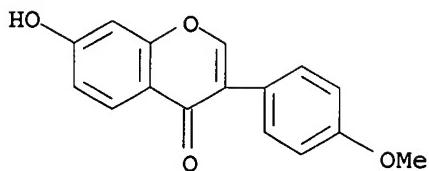
- AB The reaction of hetarylacetophenones I ($R = H, Me, Pr, 1\text{-hexyl}$; $R1 = H, OH, CO_2H$; $R2 = \text{azolyl, substituted Ph}$) with HCO_2COMe gives, under HCO_2Na catalysis, chromones II. The yield of II and the reaction rate increase with increasing π -deficiency of the hetaryl substituent or with the presence of an OH group in the C6 position of the starting acetophenone. II ($R2 = \text{azolyl}$) are formed even in the absence of catalyst.
- IT 491-80-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (attempted preparation of)
- RN 491-80-5 HCPLUS
- CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



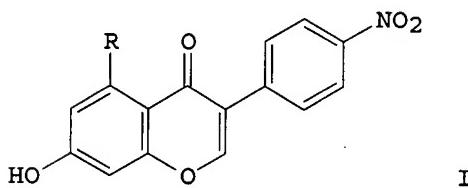
- IT 2258-42-6P, Formic acetic anhydride
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and cyclocondensation of, with hetarylacetophenones)
- RN 2258-42-6 HCPLUS
- CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac—O—CHO

- IT 485-72-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 485-72-3 HCPLUS
- CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



L15 ANSWER 5 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1992:6375 HCPLUS
 DOCUMENT NUMBER: 116:6375
 TITLE: A facile and practical preparation of
 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one
 AUTHOR(S): Liu, D. F.; Cheng, C. C.
 CORPORATE SOURCE: Cancer Cent., Univ. Kansas, Kansas City, KS, 66103,
 USA
 SOURCE: Journal of Heterocyclic Chemistry (1991), 28(6),
 1641-2
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 116:6375
 GI



AB In spite of the fact that several preparative methods for the synthesis of hydroxylated isoflavones were reported during the past fifty years, none is suitable for the preparation of isoflavones containing 5,7-dihydroxy functions.

This paper reports a simple, large scale preparation of 5,7-dihydroxy-3-(4-nitrophenyl)-4H-1-benzopyran-4-one (I, R = OH) by the condensation of the readily available 2,4,6-(HO)3C6H2COCH2C6H4NO2-4 and acetic formic anhydride in high yields. Similar isoflavones, such as I (R = H), can also be obtained in good yields in an analogous manner.

IT 2258-42-6P, Acetic formic anhydride
 RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (formation and cyclocondensation of, with phenyl(hydroxyphenyl)ethanone s)

RN 2258-42-6 HCPLUS

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac-O-CHO

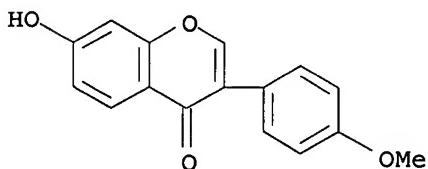
IT 485-72-3P 491-80-5P

10521972.trn

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

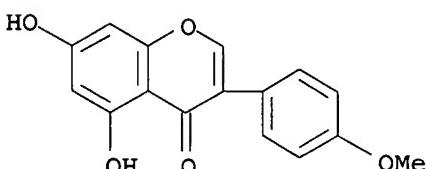
RN 485-72-3 HCPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



RN 491-80-5 HCPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



L15 ANSWER 6 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:405988 HCPLUS

DOCUMENT NUMBER: 113:5988

TITLE: Simple and effective synthesis of isoflavones and
3-arylhydroxychromones

AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Vasil'ev, S. A.

CORPORATE SOURCE: Kiev. Gos. Univ., Kiev, USSR

SOURCE: Khimiya Prirodnikh Soedinenii (1989), (5), 639-43

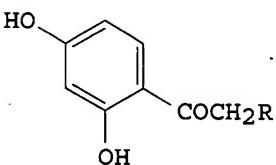
CODEN: KPSUAR; ISSN: 0023-1150

DOCUMENT TYPE: Journal

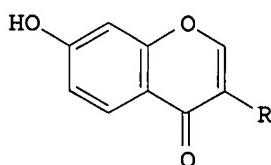
LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 113:5988

GI



I



II

AB Cyclocondensation of acetophenones I (R = substituted Ph, PhO, p-FC6H4O) with MeCO2CHO, prepared from HCO2H and CH2:C:O, gave 15-99% isoflavones II. Similarly, I react with the Vilsmeier reagent to give 95.7-98.5% II.

IT 2258-42-6P

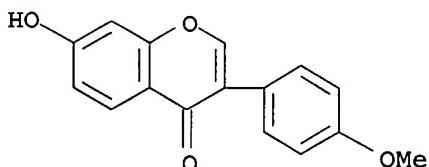
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cyclocondensation with hydroxyacetophenones, isoflavones from)

10521972.trn

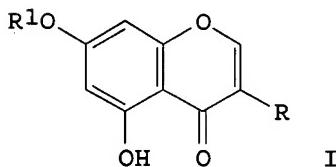
RN 2258-42-6 HCPLUS
CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

Ac-O-CHO

IT 485-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 485-72-3 HCPLUS
CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



L15 ANSWER 7 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:129748 HCPLUS
DOCUMENT NUMBER: 104:129748
TITLE: Synthesis of 5,7-dihydroxyisoflavones and their heterocyclic analogs using acetoformic anhydride
AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.
CORPORATE SOURCE: Kiiv. Derzh. Univ., Kiev, USSR
SOURCE: Dopovid Akademii Nauk Ukrains'koi RSR, Seriya B: Geologichni, Khimichni ta Biologichni Nauki (1985), (7), 44-7
DOCUMENT TYPE: CODEN: DANND6; ISSN: 0377-9785
LANGUAGE: Journal
GI Ukrainian



AB 2,4,6-(HO)3C6H2COCH2R [R = 2-pyridyl, 2-quinolyl, 2-methyl-4-thiazolyl, 5-(ethoxycarbonyl)-2-furyl, p-ClC6H4, o- and p-FC6H4, p-MeOC6H4, dihydro-6-benzodioxinyl] cyclized in the presence of HCO2Ac and either HCO2Na or Et3N to give the corresponding chromones I (R1 = H) in ≤100% yield. The intermediate I (R = heterocyclyl, R1 = HCO) were also isolated.

IT 2258-42-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization with, of aryltrihydroxyacetophenones)
RN 2258-42-6 HCPLUS

10521972.trn

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

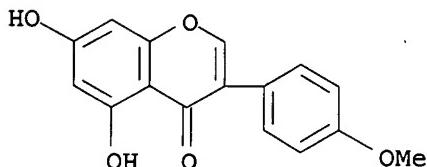
Ac—O—CHO

IT 491-80-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 491-80-5 HCPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



L15 ANSWER 8 OF 8 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1985:541792 HCPLUS

DOCUMENT NUMBER: 103:141792

TITLE: Acetic formic anhydride as a cyclizing reagent in the synthesis of isoflavones and 3-hetarylchromones

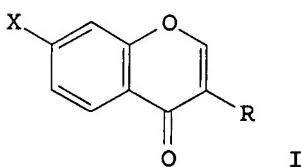
AUTHOR(S): Pivovarenko, V. G.; Khilya, V. P.; Babichev, F. S.
CORPORATE SOURCE: Kiv. Derzh. Univ., Kiev, USSR

SOURCE: Dopovid Akademii Nauk Ukrains'koi RSR, Seriya B:
Geologichni, Khimichni ta Biologichni Nauki (1985),
(4), 56-9

DOCUMENT TYPE: CODEN: DANND6; ISSN: 0377-9785

LANGUAGE: Journal
Ukrainian

GI



AB HCO₂Ac catalyzed the cyclization of 2,4-(HO)C₈H₄COCH₂R [R = 2-pyridyl, 2-and 7-quinolyl, 2-methyl-4-thiazolyl, 5-(ethoxycarbonyl)-2-furyl, C₆H₄NO₂-4, Ph, C₆H₄OMe-4, Me] in the presence of NaO₂CH or Et₃N to give ≤99% chromones I (X = HO, same R). The intermediate I (X = HCO₂; R = 2-pyridyl, 2-quinolyl, 2-methyl-4-thiazolyl) were also isolated.

IT 2258-42-6

RL: CAT (Catalyst use); USES (Uses)
(catalysts, with base, for cyclization of dihydroxyacetophenones to chromones)

RN 2258-42-6 HCPLUS

CN Acetic acid, anhydride with formic acid (CA INDEX NAME)

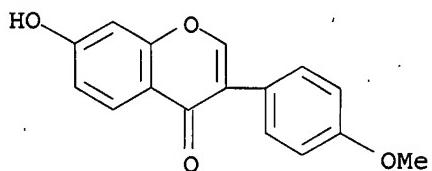
Ac—O—CHO

IT 485-72-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by cyclization of dihydroxyacetophenone derivative,
 catalysts
 for)

RN 485-72-3 HCPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-methoxyphenyl)- (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS

| | SINCE FILE | TOTAL |
|---------------------|------------|---------|
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 97.32 | 619.23 |

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | SINCE FILE | TOTAL |
|---------------------|------------|---------|
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -12.48 | -12.48 |

STN INTERNATIONAL LOGOFF AT 13:19:56 ON 10 MAY 2007